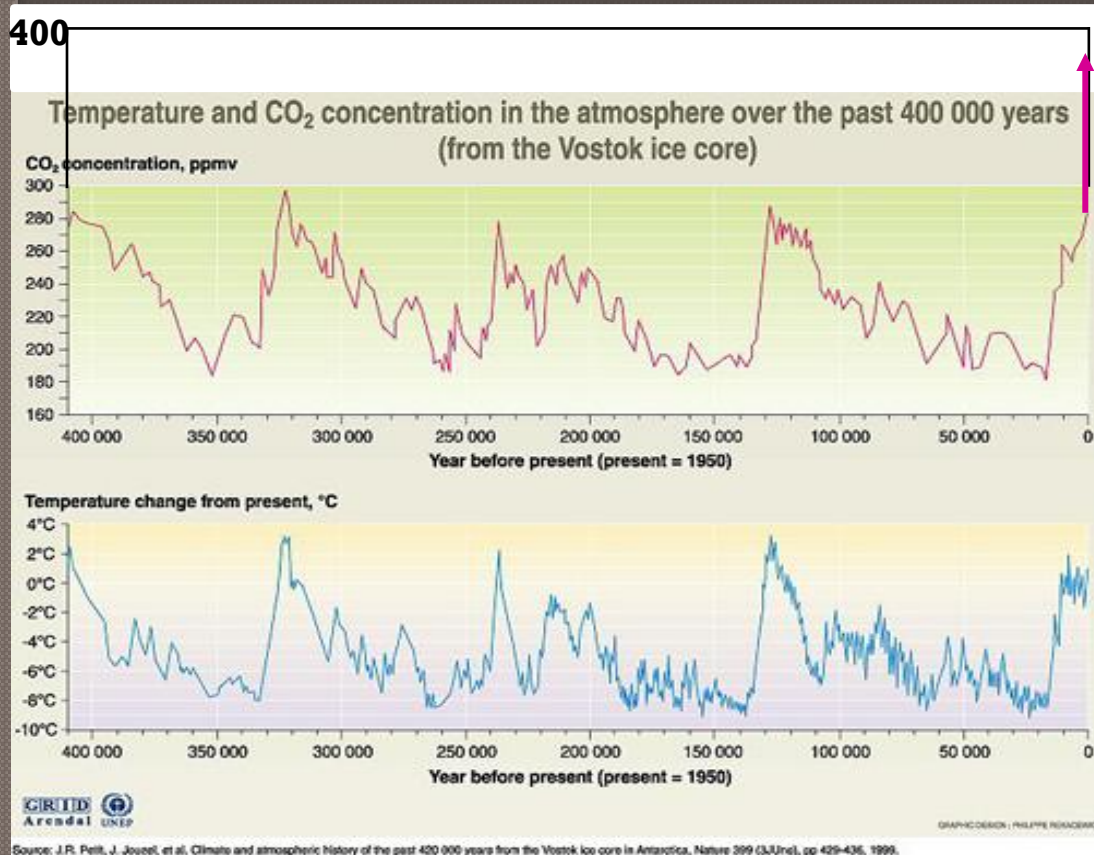


Application of NEXAFS Spectroscopy to the Carbon Sequestration Reaction

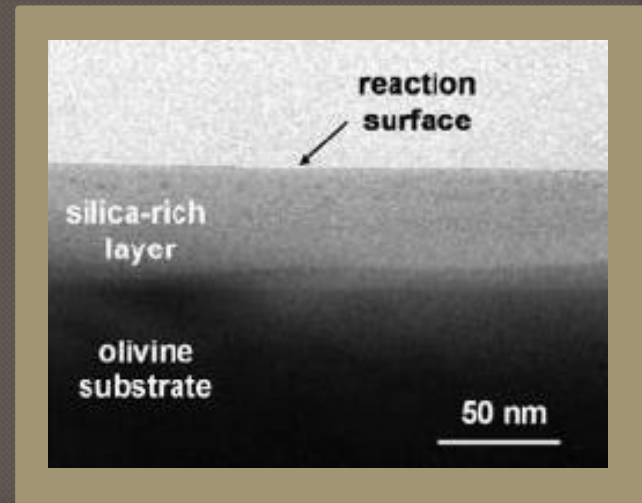


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9 March 2009**

Mineral Carbonation

- ◉ $\text{Mg}_2\text{SiO}_4 + 2\text{CO}_2 \rightleftharpoons 2\text{MgCO}_3 + \text{SiO}_2$
- ◉ Stable products
- ◉ Thermodynamically favored, very slow kinetics ($\sim 100,000$ years)
- ◉ Reaction steps to be studied
 - Dissolution of reactant mineral
 - “Passivating Layer” formation
 - Formation of product mineral

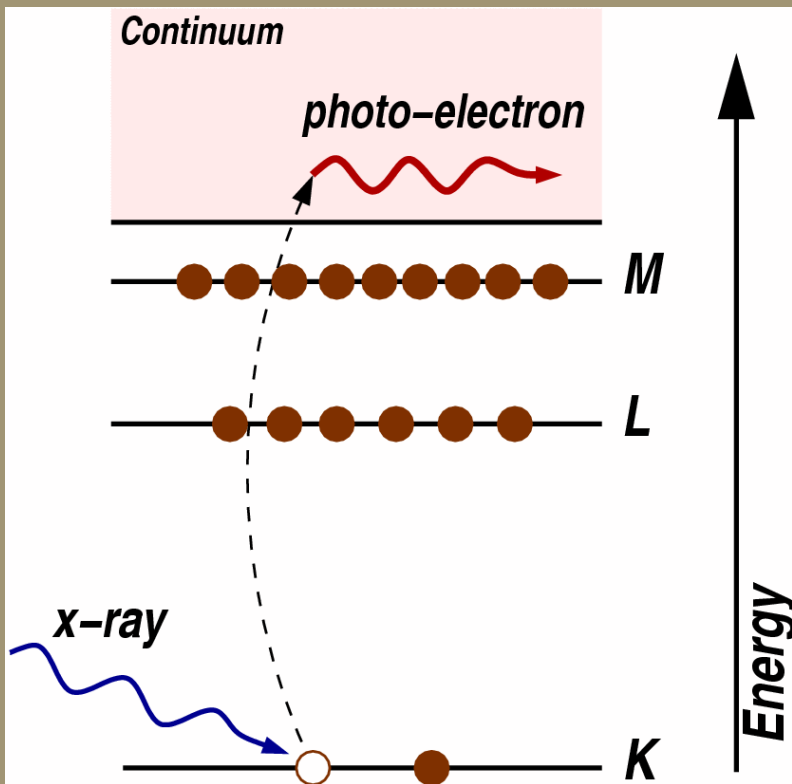
TEM image of “passivating layer”
(Bearat et al. *Environ Sci Technol.* 2006)



NEXAFS Theory

$$I = I_0 e^{-\mu t}$$

$$\mu \approx \frac{\rho Z^4}{AE^3}$$



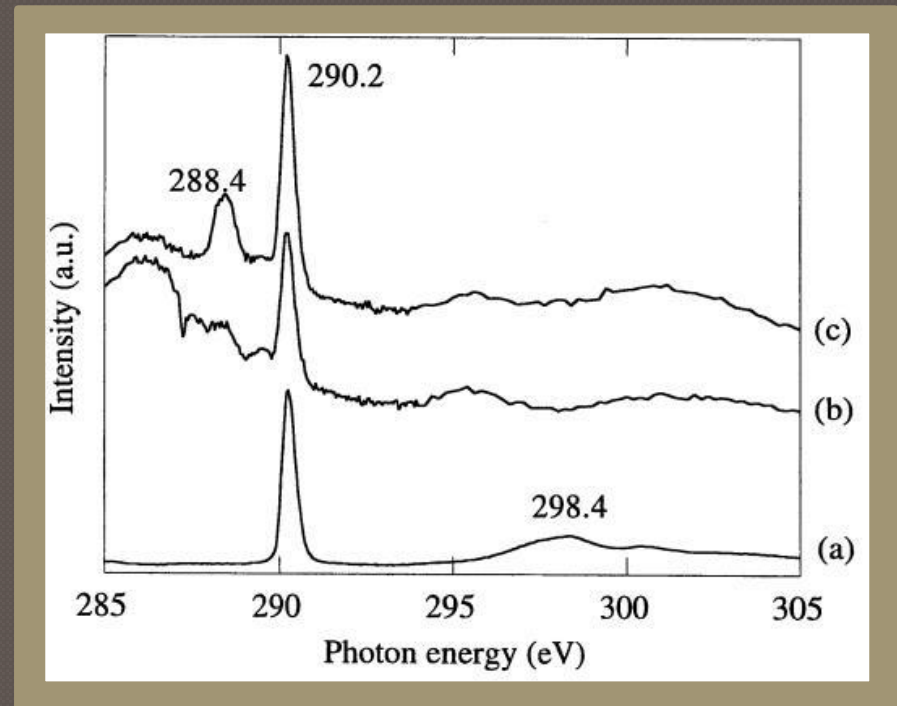
- Coordination number
 - Regular
 - Distorted octahedral
 - Tetrahedral
- Molecular orbitals
 - p – d orbital hybridization
 - Crystal field theory
- Band-structure – density of available electronic states
- Multiple-scattering – multiple bounces of the photoelectron

Application: CO₂ on MgO Surface (Carrier et al.)

● Goal: understand interaction of CO₂ and MgO(100) surface

● Results

- Evidence of MgCO₃ on surface
- Threshold pressure for carbonation
- Disordered film
- Adventitious carbon (not carbonate)



C K-edge NEXAFS spectra of (a) MgCO₃ and of MgO(100) exposed to (b) 10 Torr and (c) 175 Torr of CO₂. (Carrier et al. *Surface Review and Letters* 1999.

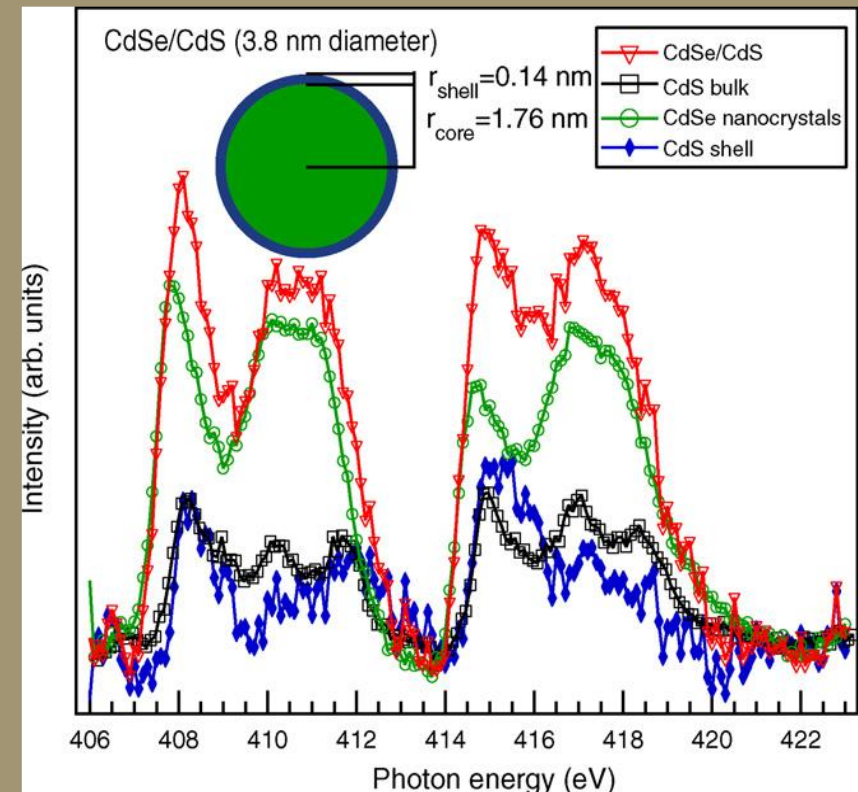
Application: Study of CdSe/CdS nanoparticles (Pietzch et al.)

○ Goal: determine the thickness of the CdS layer on the CdSe nanoparticle

○ Results

- Decomposed spectra into shell component and core component
- Determined relative volumes of shell and core

Pietzch et al. *Journal of Electron Spectroscopy and Related Phenomena*. 2008



Proposal

○ Reactant mineral dissolution

- Study interaction of water and H^+ ions with surface
- Measure Mg L2 edge to determine surface complexes that form during dissolution

○ “Passivating Layer” formation

- Probe Si K edge
- Study different Si complexes in the mineral

○ Product mineral formation

- Probe carbon K edge
- Gain information about carbonates formed and their relative abundances